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Optimal designs for regression models with autoregressive errors

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Abstract

In the one-parameter regression model with AR(1) and AR(2) errors we find explicit expressions and a continuous approximation of the optimal discrete design for the signed least square estimator. The results are used to derive the optimal variance of the best linear estimator in the continuous time model and to construct efficient estimators and corresponding optimal designs for finite samples.

Keywords: linear regression, correlated observations, signed measures, optimal design, BLUE, continuous autoregressive model

AMS Subject classification: Primary 62K05; Secondary 31A10

1. Introduction

Consider a linear regression model

$$y_j = \theta^T f(t_j) + \epsilon_j \quad (j = 1, \dots, N), \quad (1.1)$$

where $\theta \in \mathbb{R}^m$ is a vector of unknown parameters, $f(t) = (f_1(t), \dots, f_m(t))^T$ is a vector of linearly independent functions defined on some interval, say $[A, B]$, and $\epsilon_1, \dots, \epsilon_N$ are random errors with $\mathbb{E}[\epsilon_j] = 0$ for all $j = 1, \dots, N$ and covariances $\mathbb{E}[\epsilon_j \epsilon_k] = \rho(t_j - t_k)$. It is well known that the use of optimal or efficient designs yields to a reduction of costs by a statistical inference with a minimal number of experiments without loosing any accuracy. Optimal design theory has been studied intensively for the case when errors are uncorrelated using tools from convex optimization theory, see Pukelsheim (2006), but the design problem in the case of dependent data is substantially harder because the corresponding optimization problems are usually non-convex. Most authors use asymptotic arguments to construct optimal designs, which do not solve the problem of non-convexity, see for example Sacks and Ylvisaker (1966, 1968); Bickel and Herzberg (1979); N  ther (1985a); Zhigljavsky et al. (2010); Dette et al. (2015). Some optimal designs for the location model (in this case the optimization problems are in fact convex) and for a few one-parameter linear models have been discussed in Boltze and N  ther (1982); N  ther (1985a,b); P  zman and M  ller (2001) and M  ller and P  zman (2003) among others. Recently, for multi-parameter models, Dette et al. (2013) determined a necessary condition for the optimality of (asymptotic) designs for least squares estimation. Dette et al. (2014) studied

nearly universally optimal designs, while Dette et al. (2016) constructed new matrix-weighted estimators with corresponding optimal designs, which are very close to the best linear unbiased estimator with corresponding optimal designs. Although these results are promising, they rely on certain structural assumptions on the covariance kernel. For example, Dette et al. (2013) assume that the regression functions in model (1.1) are eigenfunctions of an integral operator associated with the covariance kernel of the error process and Dette et al. (2016) assume that the covariance kernel is triangular, see Mehr and McFadden (1965) for an exact definition. While these results cover the frequently used AR(1)-process as error structure, they are not applicable in models with autoregressive error processes of larger order.

The goal of the present paper is to give first insights in the optimal design problem for linear regression models with autoregressive error processes. We concentrate on a one-parameter linear regression model with an AR(1) and AR(2)-error process. In Section 2 we will introduce a signed least squares estimator and consider approximate designs on the design space $\mathcal{T} = \{t_1, \dots, t_N\}$, where the weights are not necessarily non-negative. We determine the optimal (signed) approximate design for signed least squares estimation, such that the signed least squares estimator has the same variance as the weighted least squares estimator based on observations at the experimental conditions t_1, \dots, t_N . In Section 3 we consider the one-parameter linear regression model with autoregressive errors of order 1 and study the asymptotic behavior of the signed least squares estimator with corresponding optimal design as the sample size tends to infinity. Section 4 is devoted to the case of an AR(2)-error process, where the situation is substantially more complicated. Finally, the results are illustrated on several numerical examples.

2. Various least squares estimators

For estimating θ , we use the following two estimators: the best linear unbiased estimator (BLUE)

$$\hat{\theta}_{\text{BLUE},N} = (X^T \Sigma^{-1} X)^{-1} X^T \Sigma^{-1} Y$$

and the signed least squares estimator (SLSE)

$$\hat{\theta}_{\text{SLSE},N} = (X^T \mathbf{S} X)^{-1} X^T \mathbf{S} Y, \quad (2.1)$$

where $X = (f_i(x_j))_{j,i=1}^{N,m}$ is the design matrix of size $N \times m$, \mathbf{S} is an $N \times N$ diagonal matrix with entries $+1$ and -1 on the diagonal and $\Sigma = (\rho(t_i - t_j))_{i,j=1}^N$ is the covariance matrix of observations. If \mathbf{S} is the $N \times N$ identity matrix, then SLSE coincides with the ordinary least squares estimator (LSE). The covariance matrix of the BLUE and the SLSE are given by

$$\begin{aligned} \text{Var}(\hat{\theta}_{\text{BLUE},N}) &= (X^T \Sigma^{-1} X)^{-1}, \\ \text{Var}(\hat{\theta}_{\text{SLSE},N}) &= (X^T \mathbf{S} X)^{-1} (X^T \mathbf{S} \Sigma \mathbf{S} X) (X^T \mathbf{S} X)^{-1}, \end{aligned}$$

respectively. Throughout this paper we concentrate on the one-parameter regression model

$$y_j = \theta f(t_j) + \epsilon_j, \quad (2.2)$$

and remark that an extension to the multi-parameter model (1.1) could be performed following the discussion in Dette et al. (2016). A design on the (fixed) design space $\mathcal{T} = \{t_1, \dots, t_N\}$ is an arbitrary discrete signed measure of the form $\xi = \{t_1, \dots, t_N; w_1, \dots, w_N\}$, where $w_i = s_i p_i$, $s_i \in \{-1, 1\}$, $p_i \geq 0$, $i = 1, \dots, N$, and $\sum_{i=1}^N p_i = 1$. The variance of the SLSE for the design ξ is given by

$$D(\xi) = \text{Var}(\hat{\theta}_{\text{SLSE}, N}) = \sum_{i=1}^N \sum_{j=1}^N \rho(t_i - t_j) w_i w_j f_i f_j / \left(\sum_{i=1}^N w_i f_i^2 \right)^2, \quad (2.3)$$

where we use the notation $f_i = f(t_i)$ throughout this paper. The optimal design problem consists in the minimization of this expression with respect to the weights w_1, \dots, w_N assuming that the observation points t_1, \dots, t_N are fixed. Despite the fact that the functional D in (2.3) is not convex as a function of w_1, \dots, w_N , the problem of determining the optimal weights can be easily solved by a simple application of the Cauchy-Schwarz inequality. The proof of the following lemma is given in Dette et al. (2016); see also Theorem 5.3 in N  ther (1985a), where this result was proved in a slightly different form.

Lemma 2.1. *Assume that the matrix $\Sigma = (\rho(t_i - t_j))_{i,j=1,\dots,N}$ is positive definite and $f_i \neq 0$ for all $i = 1, \dots, N$. Then the optimal weights w_1^*, \dots, w_N^* minimizing the expression (2.3) are given by*

$$w_i^* = \mathbf{e}_i^T \Sigma^{-1} \mathbf{f} / f_i; \quad i = 1, \dots, N, \quad (2.4)$$

where $\mathbf{f} = (f_1, \dots, f_N)^T$, $\mathbf{e}_i = (0, \dots, 0, 1, 0, \dots, 0)^T \in \mathbb{R}^N$ is the i -th unit vector. Moreover, for the design $\xi^* = \{t_1, \dots, t_N; w_1^*, \dots, w_N^*\}$ with weights (2.4) we have $D(\xi^*) = D^*$, where $D^* = 1/(\mathbf{f}^T \Sigma^{-1} \mathbf{f})$ is the variance of the BLUE.

Note that the optimal weights in Lemma 2.1 are not uniquely defined. In fact, they can always be multiplied by a non-zero constant without changing their optimality. In the following discussion we will consider the case where the points t_i are given by the equidistant points on the interval $[A, B]$ and the sample size N tends to infinity. Heuristically the BLUE converges in this case to the BLUE in the continuous time model, where the full trajectory of the stochastic process can be observed. Note that for any finite N the SLSE with the optimal weights defined in Lemma 2.1 has the same variance as the BLUE.

Further we study the asymptotic properties of the SLSE and the optimal weights w_i^* defined in (2.4) as the sample size increases. In many cases we will be able to approximate an N -point design $\xi = \{t_1, \dots, t_N; w_1^*, \dots, w_N^*\}$ with optimal weights defined in (2.4) by a signed measure (an approximate design) of the form

$$\xi(dt) = P_A \delta_A(dt) + P_B \delta_B(dt) + p(t) dt, \quad (2.5)$$

where $\delta_A(dt)$ and $\delta_B(dt)$ are Dirac-measures concentrated at the point A and B , respectively, and $p(\cdot)$ is a density function (not necessarily non-negative) on the interval $[A, B]$. Approximate designs of the form (2.5) are easier to understand and analyze than discrete designs of the form $\xi = \{t_1, \dots, t_N; w_1^*, \dots, w_N^*\}$, and we will illustrate in Sections 3 and 4 the derivation of the

limits in the case of autoregressive error processes of order one and two, respectively.

As already mentioned in the introduction the AR(1) process corresponds to a triangular kernel and could also be treated with methodology developed in Dette et al. (2016). We discuss it here because for this case the arguments are simpler than for the AR(2) process. In fact, for the AR(2) error process the derivation of asymptotically optimal weights w_1^*, \dots, w_N^* of the form (2.4) as the sample size tends to infinity is substantially harder.

3. Autoregressive errors of order one

Consider the regression model (1.1) with N equidistant points

$$t_j = A + (j - 1)\Delta, \quad (j = 1, \dots, N) \quad (3.1)$$

on the interval $[A, B]$, where $\Delta = (B - A)/(N - 1)$. Assume that the errors $\epsilon_1, \dots, \epsilon_N$ in (2.2) satisfy the discrete AR(1) equation

$$\epsilon_j - a\epsilon_{j-1} = z_j \quad (3.2)$$

for some $0 < a < 1$, where $\epsilon_1 \sim N(0, \sigma^2)$ and z_2, \dots, z_N are Gaussian independent identically distributed random variables with mean 0 and variance $\sigma_z^2 = (1 - a^2)\sigma^2$. Without loss of generality, we assume $\sigma^2 = 1$.

Remark 3.1. Note that discrete AR(1) processes (3.2) are often considered for the parameter $-1 < a < 1$. For the subsequent discussion we need a continuous real-valued analogue, say $\{\varepsilon(t)\}_{t \in [A, B]}$, of the discrete AR(1) error process, which is only available in the case $0 < a < 1$; see Chan and Tong (1987). The corresponding process with drift is denoted by $y(t) = \theta f(t) + \varepsilon(t)$, $t \in [A, B]$. For $-1 < a < 0$ the discrete AR(1) process (3.2) does not have a continuous real-valued analogue and therefore in this case the limiting behavior of our estimators and designs is much harder to understand.

It is also worthwhile to mention that the autocovariance function of errors $\epsilon_1, \dots, \epsilon_N$ is given by

$$\mathbb{E}[\epsilon_j \epsilon_k] = \rho(t_j - t_k) = e^{-\lambda|t_j - t_k|} = e^{\lambda t_j} e^{-\lambda t_k} \quad \text{if } t_j \leq t_k,$$

where $\lambda = -\ln(a)/\Delta$. Thus, if $a \in (0, 1)$, the AR(1) error process has a triangular covariance kernel in the sense of Mehr and McFadden (1965), and the results of Dette et al. (2016) are applicable. In the following discussion we provide a different derivation of the asymptotically optimal weights, because the arguments will be useful for the discussion of an AR(2) error process in Section 4.

For an AR(1) error process, the inverse of the covariance matrix $\Sigma = (\rho(t_i - t_j))_{i,j=1}^N$ is given by the tridiagonal matrix

$$\Sigma^{-1} = \frac{1}{S} \begin{pmatrix} 1 & k_1 & 0 & 0 & \dots \\ k_1 & k_0 & k_1 & 0 & \dots \\ 0 & k_1 & k_0 & k_1 & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots \\ & & 0 & k_1 & k_0 & k_1 \\ & & 0 & 0 & k_1 & 1 \end{pmatrix},$$

where $k_0 = 1 + a^2 = 1 + e^{-2\lambda\Delta}$, $k_1 = -a = -e^{-\lambda\Delta}$, $S = 1 - a^2 = 1 - e^{-2\lambda\Delta}$ and $\lambda = -\ln(a)/\Delta$. Recalling the definition of the optimal weights w_i^* , $i = 2, \dots, N-1$, in (2.4) we have

$$\begin{aligned} Sw_i^* f(t_i) &= k_1 f_{i-1} + k_0 f_i + k_1 f_{i+1} = (1 + a^2) f_i - a f_{i-1} - a f_{i+1} \\ &= a(2f_i - f_{i-1} - f_{i+1}) + (1 - 2a + a^2) f_i = a(2f_i - f_{i-1} - f_{i+1}) + (a - 1)^2 f_i. \end{aligned}$$

We now assume that $\lambda = -\ln(a)/\Delta$ is fixed and $\Delta = (B - A)/(N - 1) \rightarrow 0$. Since $S(\Delta) = S'(0)\Delta + o(\Delta)$ with $S'(0) = 2\lambda$ and $a = 1 - \lambda\Delta + o(\Delta)$, we obtain

$$w_i^* f(t_i) = \frac{\Delta}{S(\Delta)} \cdot \frac{a(2f_i - f_{i-1} - f_{i+1}) + (a - 1)^2 f_i}{\Delta^2} \Delta = \frac{1}{S'(0)} [-f''(t_i) + \lambda^2 f(t_i)] \Delta + o(\Delta).$$

Thus, we have $\frac{w_i^*}{\Delta} = \frac{1}{2\lambda f(t_i)} [-f''(t_i) + \lambda^2 f(t_i)] + O(\Delta)$. Therefore, for small Δ , the discrete signed measure $\{t_2, \dots, t_{N-1}; w_2^*, \dots, w_{N-1}^*\}$ is approximated by the continuous signed measure with density

$$p(t) = -\frac{1}{2\lambda f(t)} (f''(t) - \lambda^2 f(t)). \quad (3.3)$$

Now we consider the weights at the boundary points. For the left boundary weight, we obtain

$$\begin{aligned} w_1^* f(t_1) &= \frac{f_1 + k_1 f_2}{S(\Delta)} = \frac{\Delta}{S(\Delta)} \cdot \frac{f_1 - a f_2}{\Delta} = \frac{\Delta}{S(\Delta)} \left[\frac{f_1 - f_2}{\Delta} + \frac{f_2 - a f_2}{\Delta} \right] \\ &= \frac{1}{S'(0)} [-f'(t_1) - a'(0) f(t_1)] + O(\Delta). \end{aligned}$$

Since $t_1 = A$, for small Δ , we have $w_1^* \approx P_A$, where

$$P_A = \frac{1}{f(A)S'(0)} (-f'(A) - a'(0) f(A)) = \frac{1}{2\lambda f(A)} (-f'(A) + \lambda f(A)). \quad (3.4)$$

Similarly, for the right boundary weight, we obtain

$$w_N^* f(t_N) = \frac{f_N + k_1 f_{N-1}}{S(\Delta)} = \frac{\Delta}{S(\Delta)} \frac{f_N - a f_{N-1}}{\Delta} = \frac{1}{S'(0)} [f'(t_N) - a'(0) f(t_{N-1})] + O(\Delta).$$

Since $t_N = B$, for small Δ , we have $w_N^* \approx P_B$, where

$$P_B = \frac{1}{f(B)S'(0)} (f'(B) - a'(0) f(B)) = \frac{1}{2\lambda f(B)} (f'(B) + \lambda f(B)). \quad (3.5)$$

Summarizing, we have proved the following result.

Proposition 3.1. *Consider the one-parameter regression model (2.2) with AR(1) errors of the form (3.2), where $0 < a < 1$ and $f(\cdot)$ is a twice continuously differentiable function such that $f(t) \neq 0$ for all $t \in [A, B]$. For large N , the optimal discrete SLSE (defined in Lemma 2.1) is approximated by the continuous SLSE*

$$\hat{\theta} = D^* \left(P_A f(A) y(A) + P_B f(B) y(B) + \int_A^B p(t) f(t) y(t) dt \right) \quad (3.6)$$

where $D^* = \left(P_A f^2(A) + P_B f^2(B) + \int_A^B p(t) f^2(t) dt \right)^{-1}$, and $p(t)$, P_A and P_B are defined in (3.3), (3.4) and (3.5), respectively. For this approximation, we have

$$D^* = \lim_{N \rightarrow \infty} \text{Var}(\hat{\theta}_{\text{SLSE}, N}),$$

i.e. D^* is the limit of the variances (2.3) of the optimal discrete SLSE designs as $N \rightarrow \infty$.

Throughout the following discussion we call a triple (p, P_A, P_B) containing a (signed) density p and two weights P_A and P_B , an approximate design for the *continuous* SLSE defined in (3.6).

Remark 3.2. Observing the discussion in the second part of Remark 3.1 it is reasonable to compare Proposition 3.1 with Theorem 2.1 in Dette et al. (2016). Note that the expressions for the optimal signed density $p(\cdot)$ and optimal weights P_A and P_B at boundary points are particular cases of the general formulae

$$p(t) = -\frac{1}{f(t)v(t)} \left[\frac{h'(t)}{q'(t)} \right]', P_A = \frac{1}{f(A)v^2(A)q'(A)} \left[\frac{f(A)u'(A)}{u(A)} - f'(A) \right], P_B = \frac{h'(B)}{f(B)v(B)q'(B)}$$

with $u(t) = e^{\lambda t}$ and $v(s) = e^{-\lambda s}$, where $q(t) = u(t)/v(t)$ and $h(t) = f(t)/v(t)$. Indeed, we easily see that $h(t) = f(t)e^{\lambda t}$, $h'(t) = f'(t)e^{\lambda t} + f(t)\lambda e^{\lambda t}$, $q'(t) = 2\lambda e^{2\lambda t}$, $h'(t)/q'(t) = f'(t)e^{-\lambda t} + f(t)\lambda e^{-\lambda t}$ and, consequently,

$$\begin{aligned} p(t) &= -\frac{1}{f(t)e^{-\lambda t}} (f'(t)e^{-\lambda t} + f(t)\lambda e^{-\lambda t})' \\ &= -\frac{f''(t)e^{-\lambda t} - \lambda f''(t)e^{-\lambda t} + f'(t)\lambda e^{-\lambda t} - f(t)\lambda^2 e^{-\lambda t}}{f(t)e^{-\lambda t}} = -\frac{1}{2\lambda f(t)} (f''(t) - \lambda^2 f(t)). \end{aligned}$$

as desired. Similarly, we have

$$\begin{aligned} P_A &= \frac{1}{f(A)e^{-2\lambda A} 2\lambda e^{2\lambda A}} \left[\frac{f(A)\lambda e^{\lambda A}}{e^{\lambda A}} - f'(A) \right] = \frac{1}{2\lambda f(A)} (-f'(A) + \lambda f(A)) \\ P_B &= \frac{f'(B)e^{\lambda B} + f(B)\lambda e^{\lambda B}}{f(B)e^{-\lambda B} 2\lambda e^{2\lambda B}} = \frac{1}{2\lambda f(B)} (f'(B) + \lambda f(B)). \end{aligned}$$

4. Autoregressive errors of order two

In this section we assume that the observations in model (2.2) are taken at N equidistant points of the form (3.1) and that the errors $\epsilon_1, \dots, \epsilon_N$ satisfy the discrete AR(2) equation

$$\epsilon_j - a_1 \epsilon_{j-1} - a_2 \epsilon_{j-2} = z_j, \quad (4.1)$$

where z_j are Gaussian independent identically distributed random variables with mean 0 and variance $\sigma_z^2 = \sigma^2(1 + a_2)((1 - a_2^2) - a_1^2)/(1 - a_2)$. Here we make a usual assumption that (4.1) defines the AR(2) process for $j \in \{\dots, -2, -1, 0, 1, 2, \dots\}$ but we only take the values such that $j \in \{1, 2, \dots, N\}$. Note that the AR(2) process is often considered for parameters a_1 and

a_2 satisfying the following three inequalities: $a_2 + a_1 < 1$, $a_2 - a_1 < 1$ and $|a_2| < 1$ (these inequalities ensure that the AR(2) process is causal). Since we need a continuous real-valued analogue for the discrete AR(2) process, we will assume that parameters in (4.1) satisfy stricter inequalities: $a_2 + a_1 < 1$, $-1 < a_2 < 0$ and $a_1 > 0$.

Let $r_k = \mathbb{E}[\epsilon_j \epsilon_{j+k}]$ be the autocovariance function of the AR(2) process $\{\epsilon_1, \dots, \epsilon_N\}$ and assume without loss of generality that $\sigma^2 = 1$. The inverse of the covariance matrix $\Sigma = (\mathbb{E}[\epsilon_j \epsilon_k])_{j,k}$ of the discrete AR(2) process is the five-diagonal matrix

$$\Sigma^{-1} = \frac{1}{S} \begin{pmatrix} k_{11} & k_{12} & k_2 & 0 & 0 & 0 & \dots \\ k_{21} & k_{22} & k_1 & k_2 & 0 & 0 & \dots \\ k_2 & k_1 & k_0 & k_1 & k_2 & 0 & \dots \\ 0 & k_2 & k_1 & k_0 & k_1 & k_2 & \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\ & & 0 & k_2 & k_1 & k_0 & k_1 & k_2 \\ & & 0 & 0 & k_2 & k_1 & k_{22} & k_{12} \\ & & 0 & 0 & 0 & k_2 & k_{21} & k_{11} \end{pmatrix} \quad (4.2)$$

where the non-vanishing elements are given by $k_0 = 1 + a_1^2 + a_2^2$, $k_1 = -a_1 + a_1 a_2$, $k_2 = -a_2$, $k_{11} = 1$, $k_{12} = k_{21} = -a_1$, $k_{22} = 1 + a_1^2$ and $S = (1 + a_1 - a_2)(1 - a_1 - a_2)(1 + a_2)/(1 - a_2)$. Using Lemma 2.1 and the explicit form (4.2) for Σ^{-1} we straightforwardly obtain the explicit expressions for the optimal weights w_i^* defined in (2.4).

To derive asymptotic approximations for w_i^* , we have to study the behavior of w_i^* in dependence on the autocovariance function r_k of the AR(2) process (4.1). There are three different types of autocovariance functions which we consider below.

Formally, a continuous AR(2) process is a solution of the linear stochastic differential equation of the form

$$d\varepsilon'(t) = \tilde{a}_1 \varepsilon'(t) + \tilde{a}_2 \varepsilon(t) + \sigma_0^2 dW(t),$$

where $W(t)$ is a standard Wiener process, see Brockwell et al. (2007). Note that the process $\varepsilon(t)$ has the continuous derivative $\varepsilon'(t)$ and the continuous process with drift is again denoted by $y(t) = \theta f(t) + \varepsilon(t)$, $t \in [A, B]$. We also note that $y(t)$ is differentiable on the interval $[A, B]$. There are three different forms of the autocovariance function (note that we assume throughout $\sigma^2 = 1$) of continuous AR(2) processes, see e.g. formulas (14)–(16) in He and Wang (1989):

$$\rho^{(1)}(t) = \frac{\lambda_2}{\lambda_2 - \lambda_1} e^{-\lambda_1 |t|} - \frac{\lambda_1}{\lambda_2 - \lambda_1} e^{-\lambda_2 |t|}, \quad (4.3)$$

where $\lambda_1 \neq \lambda_2$, $\lambda_1 > 0$, $\lambda_2 > 0$,

$$\rho^{(2)}(t) = e^{-\lambda |t|} \left\{ \cos(q|t|) + \frac{\lambda}{q} \sin(q|t|) \right\},$$

where $\lambda > 0$, $q > 0$, and

$$\rho^{(3)}(t) = e^{-\lambda |t|} (1 + \lambda |t|),$$

where $\lambda > 0$. From formulas (11)–(13) in He and Wang (1989) we obtain that the corresponding three forms of the autocovariances of the discrete AR(2) process (4.1) are:

$$r_k^{(1)} = \mathbb{E}[\epsilon_j \epsilon_{j+k}] = Cp_1^k + (1 - C)p_2^k, \quad C = \frac{(1 - p_2^2)p_1}{(1 - p_2^2)p_1 - (1 - p_1^2)p_2}, \quad (4.4)$$

where $j \geq 0$, $p_1 \neq p_2$, $0 < |p_1|, |p_2| < 1$,

$$r_k^{(2)} = p^k (\cos(bk) + C \sin(bk)), \quad C = \cot(b) \frac{1 - p^2}{1 + p^2}, \quad (4.5)$$

where $0 < p < 1$, $0 < b < 2\pi$ and $b \neq \pi$, and

$$r_k^{(3)} = p^k (1 + kC), \quad C = \frac{1 - p^2}{1 + p^2}, \quad (4.6)$$

where $0 < |p| < 1$. We determine approximations for the optimal weights w_i^* in Lemma 2.1 for the three different types of autocovariance functions. All results are summarized in Theorem 4.1 below. The proof is somewhat similar (but more difficult) to the derivation above presented for the AR(1) errors.

Theorem 4.1. *Consider the one-parameter model (2.2) such that the errors follow the AR(2) equation. Assume that $f(\cdot)$ is a four times continuously differentiable and $f(t) \neq 0$ for all $t \in [A, B]$. Define the following constants depending on the form of the autocovariance function r_k . If r_k is of the form (4.4), set*

$$\begin{aligned} \lambda_1 &= -\frac{\ln(p_1)}{\Delta}, \quad \lambda_2 = -\frac{\ln(p_2)}{\Delta}, \quad \tau_0 = \lambda_1^2 \lambda_2^2, \quad \tau_2 = \lambda_1^2 + \lambda_2^2, \quad \beta_1 = \lambda_1 + \lambda_2, \quad \beta_0 = \lambda_1 \lambda_2, \\ \gamma_1 &= \lambda_1^2 + \lambda_1 \lambda_2 + \lambda_2^2, \quad \gamma_0 = \lambda_1 \lambda_2 (\lambda_1 + \lambda_2), \quad s_3 = 2\lambda_1 \lambda_2 (\lambda_1 + \lambda_2). \end{aligned}$$

If r_k is of the form (4.5), set

$$\begin{aligned} \lambda &= -\frac{\ln(p)}{\Delta}, \quad q = -\frac{b}{\Delta}, \quad \tau_0 = (\lambda^2 + q^2)^2, \quad \tau_2 = 2(\lambda^2 - q^2), \quad \beta_1 = 2\lambda, \quad \beta_0 = \lambda^2 + q^2, \\ \gamma_1 &= (3\lambda^2 - q^2), \quad \gamma_0 = 2\lambda(\lambda^2 + q^2), \quad s_3 = 4\lambda(\lambda^2 + q^2). \end{aligned}$$

If r_k is of the form (4.6), set

$$\lambda = -\frac{\ln(p)}{\Delta}, \quad \tau_0 = \lambda^4, \quad \tau_2 = 2\lambda^2, \quad \beta_1 = 2\lambda, \quad \beta_0 = \lambda^2, \quad \gamma_1 = 3\lambda^2, \quad \gamma_0 = 2\lambda^3, \quad s_3 = 4\lambda^3.$$

For large N , the optimal discrete SLSE (defined in Lemma 2.1) can be approximated by the continuous SLSE

$$\hat{\theta} = D^* (Q_B f(B) y'(B) - Q_A f(A) y'(A) + P_A f(A) y(A) + P_B f(B) y(B) + \int_A^B p(t) f(t) y(t) dt)$$

where

$$D^* = \left(Q_B f(B) f'(B) - Q_A f(A) f'(A) + P_A f^2(A) + P_B f^2(B) + \int_A^B p(t) f^2(t) dt \right)^{-1}.$$

For this approximation, we have $D^* = \lim_{N \rightarrow \infty} \text{Var}(\hat{\theta}_{SLSE,N})$, i.e. D^* is the limit of the variance (2.3) of the optimal discrete SLSE design as $N \rightarrow \infty$. Here the quantities $p(t)$, Q_A , Q_B , P_A and P_B in the continuous SLSE are defined by

$$p(t) = -\frac{1}{s_3 f(t)} (\tau_2 f''(t) - \tau_0 f(t) - f'''(t)), \quad (4.7)$$

$$P_A = \frac{1}{s_3 f(A)} (f'''(A) - \gamma_1 f'(A) + \gamma_0 f(A)),$$

$$P_B = \frac{1}{s_3 f(B)} (-f'''(B) + \gamma_1 f'(B) + \gamma_0 f(B)),$$

$$Q_A = \frac{1}{s_3 f(A)} (f''(A) - \beta_1 f'(A) + \beta_0 f(A)),$$

$$Q_B = \frac{1}{s_3 f(B)} (f''(B) + \beta_1 f'(B) + \beta_0 f(B)). \quad (4.8)$$

5. Examples

5.1. Approximations of the discrete SLSE

Consider the one-parameter model with $f(t) = t^\alpha$ and AR(1) errors. The design space is an interval $[A, B]$ such that $f(t) \neq 0$ for all $t \in [A, B]$. Then the optimal discrete design for the SLSE is approximated by a design of the form (2.5), where the density $p(t)$, and the weights P_A and P_B are defined by

$$p(t) = -\frac{1}{2\lambda} (\alpha(\alpha-1)t^{-2} - \lambda^2), \quad P_A = \frac{1}{2\lambda} (-\alpha A^{-1} + \lambda), \quad P_B = \frac{1}{2\lambda} (\alpha B^{-1} + \lambda).$$

In Table 1 we display values of $p(t)$, $P(A)$ and P_B for several exponents α and also for the regression function $f(t) = e^t$. For example, if $f(t) = e^t$ we observe that P_A is positive for $\lambda > 1$ and negative for $0 < \lambda < 1$, P_B is positive for $\lambda > 0$, $p(t)$ is positive for $\lambda > 1$ and negative for $\lambda \in (0, 1)$. For large λ , the contribution of observations at the interval (A, B) to the continuous SLSE is significant. For the location model $f(t) = 1$, we can see that $P_B = P_B = 1/2$ and $p(t) = \lambda/2$. This implies that for small λ the contribution of observations at boundary points to the continuous SLSE is large and the contribution of observations at the interval (A, B) to the continuous SLSE is small. For large λ , the contribution of observations at the interval (A, B) to the continuous SLSE is essential.

Next we consider the same models with an AR(2) error process. If $f(t) = t^\alpha$ then SLSE is approximated by the continuous SLSE of the form (2.5), where

$$p(t) = -\frac{1}{s_3} (\tau_2 \alpha(\alpha-1)t^{-2} - \tau_0 - \alpha(\alpha-1)(\alpha-2)(\alpha-3)t^{-4}),$$

$P_A = \frac{1}{s_3} (\alpha(\alpha-1)(\alpha-2)A^{-3} - \gamma_1 \alpha A^{-1} + \gamma_0)$, $P_B = \frac{1}{s_3} (-\alpha(\alpha-1)(\alpha-2)B^{-3} + \gamma_1 \alpha B^{-1} + \gamma_0)$, $Q_A = \frac{1}{s_3} (\alpha(\alpha-1)A^{-2} - \beta_1 \alpha A^{-1} + \beta_0)$, $Q_B = \frac{1}{s_3} (\alpha(\alpha-1)B^{-2} + \beta_1 \alpha B^{-1} + \beta_0)$. Note that signs of $p(t)$, Q_A , Q_B , P_A and P_B depend on the form of the autocovariance function and its parameters. For the form (4.6), we provide values of $p(t)$, Q_A , Q_B , P_A and P_B for several functions $f(t)$ in Table 2. The other cases can be obtained similarly and are not displayed for the sake of brevity.

Table 1: The function $p(t)$ and the weights P_A and P_B of the continuous SLSE for several functions $f(t)$ and an AR(1) error process.

$f(t)$	P_A	P_B	$p(t)$
1	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{\lambda}{2}$
t	$\frac{1}{2} - \frac{1}{2A\lambda}$	$\frac{1}{2} + \frac{1}{2B\lambda}$	$\frac{\lambda}{2}$
t^2	$\frac{1}{2} - \frac{1}{A\lambda}$	$\frac{1}{2} + \frac{1}{B\lambda}$	$\frac{\lambda}{2} - \frac{1}{\lambda t^2}$
t^3	$\frac{1}{2} - \frac{3}{2A\lambda}$	$\frac{1}{2} + \frac{3}{2B\lambda}$	$\frac{\lambda}{2} - \frac{\lambda t^2}{3}$
t^4	$\frac{1}{2} - \frac{2}{A\lambda}$	$\frac{1}{2} + \frac{2}{B\lambda}$	$\frac{\lambda}{2} - \frac{6}{\lambda t^2}$
e^t	$\frac{1}{2} - \frac{1}{2\lambda}$	$\frac{1}{2} + \frac{1}{2\lambda}$	$\frac{\lambda}{2} - \frac{1}{2\lambda}$

For example, if $f(t) = e^t$ we can see that both P_A and Q_A are positive for all $\lambda \neq 1$, P_B is positive for $\lambda > 0.5$ and negative for $\lambda \in (0, 0.5)$, $p(t)$ is positive for $\lambda > \sqrt{2}$ and negative for $\lambda \in (0, \sqrt{2})$. For large λ , the contribution of observations at the interval (A, B) to the continuous SLSE is notable. For the location model $f(t) = 1$, we can see that $P_A = P_B = 1/2$, $Q_A = Q_B = 1/(4\lambda)$ and $p(t) = \lambda/4$. This implies that for small λ the contribution of observations at boundary points to the continuous SLSE is very large and the contribution of observations at the interval (A, B) to the continuous SLSE is small. For large λ , the contribution of observations at the interval (A, B) to the continuous SLSE is essential.

Table 2: The function $p(t)$ and the weights P_A , P_B , Q_A and Q_B in the continuous SLSE for several functions $f(t)$ and an AR(2) error process with the autocovariance function (4.6).

$f(t)$	P_A	P_B	$p(t)$	Q_A	Q_B
1	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{\lambda}{4}$	$\frac{1}{4\lambda}$	$\frac{1}{4\lambda}$
t	$\frac{1}{2} - \frac{3}{4A\lambda}$	$\frac{1}{2} + \frac{3}{4B\lambda}$	$\frac{\lambda}{4}$	$\frac{1}{4\lambda} - \frac{1}{2A\lambda^2}$	$\frac{1}{4\lambda} + \frac{1}{2B\lambda^2}$
t^2	$\frac{1}{2} - \frac{3}{2A\lambda}$	$\frac{1}{2} + \frac{3}{2B\lambda}$	$\frac{\lambda}{4} - \frac{1}{\lambda t^2}$	$\frac{1}{4\lambda} - \frac{1}{A\lambda^2} + \frac{1}{2A^2\lambda^3}$	$\frac{1}{4\lambda} + \frac{1}{B\lambda^2} + \frac{1}{2B^2\lambda^3}$
t^3	$\frac{1}{2} - \frac{9}{4A\lambda} + \frac{3}{2A^3\lambda^3}$	$\frac{1}{2} + \frac{9}{4B\lambda} - \frac{3}{2B^3\lambda^3}$	$\frac{\lambda}{4} - \frac{3}{\lambda t^2}$	$\frac{1}{4\lambda} - \frac{3}{2A\lambda^2} + \frac{3}{2A^2\lambda^3}$	$\frac{1}{4\lambda} + \frac{3}{2B\lambda^2} + \frac{3}{2B^2\lambda^3}$
t^4	$\frac{1}{2} - \frac{3}{A\lambda} + \frac{6}{A^3\lambda^3}$	$\frac{1}{2} + \frac{3}{B\lambda} - \frac{6}{B^3\lambda^3}$	$\frac{\lambda}{4} - \frac{6}{\lambda t^2} + \frac{6}{\lambda^3 t^4}$	$\frac{1}{4\lambda} - \frac{2}{A\lambda^2} + \frac{3}{A^2\lambda^3}$	$\frac{1}{4\lambda} + \frac{2}{B\lambda^2} + \frac{3}{B^2\lambda^3}$
e^t	$\frac{1}{2} - \frac{3}{4\lambda} + \frac{1}{4\lambda^3}$	$\frac{1}{2} + \frac{3}{4\lambda} - \frac{1}{4\lambda^3}$	$\frac{\lambda}{4} - \frac{1}{2\lambda} + \frac{1}{4\lambda^3}$	$\frac{1}{4\lambda} - \frac{1}{2\lambda^2} + \frac{1}{4\lambda^3}$	$\frac{1}{4\lambda} + \frac{1}{2\lambda^2} + \frac{1}{4\lambda^3}$

5.2. Practical implementation

Suppose that the N equidistant points defined in (3.1) are the potential observation points. Let $K + 2$ be the number of observations actually taken in the experiment and that we want to construct a discrete design, which can be implemented in practice. If K is small and N is large, then efficient designs and corresponding estimators for the model (2.2) can be derived from the continuous approximations, which have been developed in the previous sections.

In Dette et al. (2016) a procedure with a good finite sample performance is proposed. It consists of a slight modification of the SLSE given in (2.1) and a discretization of the density $p(t)$ defined in (3.3) for AR(1) errors and (4.8) for AR(2) errors. To be precise consider a continuous SLSE with weights at the points A and B (the end-points of the interval $[A, B]$), which correspond

to the masses P_A and P_B and, for the AR(2) errors, Q_A and Q_B as well. We thus only need to approximate the continuous part of the design, which has a density on (A, B) , by a K -point design with equal masses.

We assume that the density $p(\cdot)$ is not identically zero on the interval (A, B) . Define $\varphi(t) = \kappa|p(t)|$ for $t \in (A, B)$ and choose the constant κ such that $\int_A^B \varphi(t)dt = 1$, that is, $\kappa = 1/\int_A^B |p(t)|dt$. Denote by $F(t) = \int_A^t \varphi(s)ds$ the corresponding cumulative distribution function. As K -point design we use a K -point approximation to the measure with density $\varphi(t)$, that is $\hat{\xi}_K = \{t_{1,K}, \dots, t_{K,K}; 1/K, \dots, 1/K\}$, where $t_{i,K} = R(F^{-1}(i/(K+1)))$ $i = 1, 2, \dots, K$. Here $R(t)$ is the operator of rounding a number t towards the set of points defined by (3.1); that is, points $R(F(i/(K+1))) = t_{i,K} := A + (\nu_i - 1)\Delta$. For given i , ν_i is defined from

$$|F(i/(K+1)) - A + (\nu_i - 1)\Delta| = \min\{|F(i/(K+1)) - A + (j-1)\Delta|; j = 1, \dots, N\}.$$

If $p(t) = 0$ on a sub-interval of $[A, B]$ and $F^{-1}(i/(K+1))$ is not uniquely defined then we choose the smallest element from the set $R(F^{-1}(i/(K+1)))$ as $t_{i,K}$. Also we define $s_{i,K} = \text{sign}(p(t_{i,K}))$ and obtain from the representation of the continuous SLSE for AR(1) errors in Proposition 3.1 a reasonable estimator with corresponding design. To be precise, y_1, \dots, y_{K+2} should be observed at experimental conditions $A, t_{1,K}, t_{2,K}, \dots, t_{K,K}, B$, respectively, and the parameter θ has to be estimated by the following modified SLSE

$$\hat{\theta}_{K+2} = D_{K+2} \left(P_A f(A) y_A + P_B f(B) y_B + \frac{B-A}{\kappa K} \sum_{i=1}^K s_{i,K} f(t_{i,K}) y_i \right),$$

where

$$D_{K+2} = \left(P_A f^2(A) + P_B f^2(B) + \frac{B-A}{\kappa K} \sum_{i=1}^K s_{i,K} f^2(t_{i,K}) \right)^{-1}.$$

It follows from the discussion of the previous paragraph that $\text{Var}(\hat{\theta}_{K+2}) \approx D^*$, where D^* is defined in (3.6). Similarly, the modified SLSE for AR(2) errors is defined by

$$\begin{aligned} \hat{\theta}_{K+2} = D_{K+2} & \left(Q_B f(B) y'(B) - Q_A f(A) y'(A) \right. \\ & \left. + P_A f(A) y_A + P_B f(B) y_B + \frac{B-A}{\kappa K} \sum_{i=1}^K s_{i,K} f(t_{i,K}) y(t_{i,K}) \right) \end{aligned} \quad (4.9)$$

where

$$D_{K+2} = \left(Q_B f(B) f'(B) - Q_A f(A) f'(A) + P_A f^2(A) + P_B f^2(B) + \frac{B-A}{\kappa K} \sum_{i=1}^K s_{i,K} f^2(t_{i,K}) \right)^{-1}.$$

Note that the expression in (4.9) contains the derivatives $y'(A)$ and $y'(B)$ of the observed process $\{y(t)\}_{t \in [A, B]}$. If these derivatives are not available then we recommend to make two additional observations at the points $A + \Delta$ and $B - \Delta$ and to replace the derivatives by their

approximations $(y_{A+\Delta} - y_A)/\Delta$ and $(y_B - y_{B-\Delta})/\Delta$. Thus, we replace the estimator (4.9) by the weighted least squares estimator (WLSE)

$$\tilde{\theta}_{K+4} = (X^T W X)^{-1} X^T W Y, \quad (4.10)$$

where $Y = (y_A, y_{A+\Delta}, y_{t_{1,K}}, \dots, y_{t_{K,K}}, y_{B-\Delta}, y_B)^T$ and the matrix W is defined by

$$W = \text{diag}\left\{\frac{P_A}{2} + \frac{Q_A}{\Delta}, \frac{P_A}{2} - \frac{Q_A}{\Delta}, s_{1,K} \frac{B-A}{\kappa K}, \dots, s_{K,K} \frac{B-A}{\kappa K}, \frac{P_B}{2} - \frac{Q_B}{\Delta}, \frac{P_B}{2} + \frac{Q_B}{\Delta}\right\}. \quad (4.11)$$

Note that the variance of $\tilde{\theta}_{K+4}$ is given by $\text{Var}(\tilde{\theta}_{K+4}) = (X^T W X)^{-1} (X^T W \Sigma W X) (X^T W X)^{-1}$.

5.3. Practical performance

Consider the regression model (2.2) with $f(t) = 1$, $[A, B] = [0, 1]$ and AR(2) errors. Suppose that $N = 101$ so that $t_i = i/100$, $i = 0, 1, \dots, N$, are potential observation points. We also assume that the autocorrelation function r_k is of the form (4.6) with $\lambda = 1$. We investigate the design ξ_{K+2} with $(K+2)$ points $0, t_{1,K}, t_{2,K}, \dots, t_{K,K}, 1$ and the design ξ_{K+4} with $(K+4)$ points $0, 0.01, t_{1,K}, t_{2,K}, \dots, t_{K,K}, 0.99, 1$. The points $t_{1,K}, t_{2,K}, \dots, t_{K,K}$ are shown in the second column of Table 3. In this table we also display the variances of the WLSE $\tilde{\theta}_{K+4}$, defined by (4.11), the LSE $\hat{\theta}_{\text{LSE}, K+2}$ based on the design ξ_{K+2} and the BLUE $\hat{\theta}_{\text{BLUE}, K+2}$ and $\hat{\theta}_{\text{BLUE}, K+4}$ for the designs ξ_{K+2} and ξ_{K+4} , respectively. Let $\hat{\theta}_{\text{BLUE}}$ denote the BLUE based on 101 observations at the points $\{i/100 \mid i = 0, \dots, 100\}$, then we observe $0.80158449 = \text{Var}(\hat{\theta}_{\text{BLUE}}) \approx D^* = 0.8$, which is in agreement with Theorem 4.1. We also observe $\text{Var}(\hat{\theta}_{\text{BLUE}, K+4}) \cong \text{Var}(\hat{\theta}_{\text{BLUE}})$ and $\text{Var}(\hat{\theta}_{\text{BLUE}, K+2}) \not\cong \text{Var}(\hat{\theta}_{\text{BLUE}})$ showing the importance of taking one additional observation at each boundary point A and B . Note that the proposed estimator $\tilde{\theta}_{K+4}$ defined in (4.11) is nearly as accurate as the BLUE $\hat{\theta}_{\text{BLUE}, K+4}$ at the same points and that the LSE $\hat{\theta}_{\text{LSE}, K+2}$ is about 10 – 15% worse than the BLUE.

Table 3: The variances of the LSE, the WLSE defined by (4.11) and the BLUE for designs with $K+2$ and $K+4$ points. $f(t) = 1$, $[A, B] = [0, 1]$, $N = 101$, the autocovariance structure is given by (4.6) with $\lambda = 1$, which yields $D^* = 0.80000$ and $\text{Var}(\hat{\theta}_{\text{BLUE}}) = 0.80158449$.

K	$t_{1,K}, \dots, t_{K,K}$	$\text{Var}(\hat{\theta}_{\text{LSE}, K+2})$	$\text{Var}(\tilde{\theta}_{K+4})$	$\text{Var}(\hat{\theta}_{\text{BLUE}, K+2})$	$\text{Var}(\hat{\theta}_{\text{BLUE}, K+4})$
2	0.33, 0.67	0.914	0.80170	0.82663	0.80158714
3	0.25, 0.5, 0.75	0.921	0.80165	0.82022	0.80158533
4	0.2, 0.4, 0.6, 0.8	0.925	0.80162	0.81681	0.80158484
5	0.17, 0.33, 0.5, 0.67, 0.83	0.928	0.80161	0.81443	0.80158466

As a second example, consider the regression model (2.2) with $f(t) = t^2$, $[A, B] = [0.1, 1.1]$ and AR(2) errors. Suppose that $N = 101$ so that $t_i = 0.1 + i/100$, $i = 0, 1, \dots, N$, are potential observation points. We also assume that the autocorrelation function r_j is of the form (4.6) with $\lambda = 2$. We investigate the design ξ_{K+2} with $(K+2)$ points $0.1, t_{1,K}, t_{2,K}, \dots, t_{K,K}, 1.1$ and the design ξ_{K+4} with $(K+4)$ points $0.1, 0.11, t_{1,K}, t_{2,K}, \dots, t_{K,K}, 1.09, 1.1$. The non-trivial points

are shown in the second column of Table 4. In the other columns we display the variances of the different estimators introduced in the previous paragraph. We observe, similarly to the previous example, $0.37055791 = \text{Var}(\hat{\theta}_{\text{BLUE}}) \approx D^* = 0.36543$ which is again in line with Theorem 4.1. Note also $\text{Var}(\hat{\theta}_{\text{BLUE},K+4}) \cong \text{Var}(\hat{\theta}_{\text{BLUE}})$ and the estimator $\hat{\theta}_{\text{BLUE},K+2}$ without the two additional observations at the boundary is not efficient. Again the proposed estimator $\tilde{\theta}_{K+4}$ is nearly as accurate as the BLUE at the same points but the LSE $\hat{\theta}_{\text{LSE},K+2}$ is dramatically worse than the BLUE.

Table 4: *The variances of the LSE, the WLSE and the BLUE for designs with $K + 2$ and $K + 4$ points. $f(t) = t^2$, $[A, B] = [0.1, 1.1]$, $N = 101$ and the autocovariance is given by (4.6) with $\lambda = 2$, which yields $D^* = 60000/164189 \cong 0.36543$ and $\text{Var}(\hat{\theta}_{\text{BLUE}}) = 0.37055791$.*

K	$t_{1,K}, \dots, t_{K,K}$	$\text{Var}(\hat{\theta}_{\text{LSE},K+2})$	$\text{Var}(\tilde{\theta}_{K+4})$	$\text{Var}(\hat{\theta}_{\text{BLUE},K+2})$	$\text{Var}(\hat{\theta}_{\text{BLUE},K+4})$
2	0.14, 0.22	0.723	0.40218	0.53175	0.37079053
3	0.12, 0.17, 0.27	0.751	0.40204	0.52509	0.37072082
4	0.12, 0.15, 0.20, 0.30	0.783	0.40176	0.52089	0.37068565
5	0.12, 0.14, 0.17, 0.22, 0.33	0.818	0.40139	0.51689	0.37065785

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